

Formaldehyde

50-00-0 | DTXSID7020637

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.39e-01

Global applicability domain: Inside

Local applicability domain index: 4.94e-01

Confidence level: 7.10e-01

Nearest Neighbors from the Training Set

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N,N-Dimethylformamide

Measured: -0.100

Predicted: 4.94e-02

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1,4-Dioxane

Measured: -0.300

Predicted: 2.70e-02

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Morpholine

Measured: 0.45

Predicted: 2.71e-01

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Piperazine

Measured: 0.59

Predicted: 3.88e-01

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Furan

Measured: 0.7

Predicted: 6.89e-01